



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Recovery and Reinvestment Act

-- Status of ASCR Projects --

ASCAC Meeting
Washington, DC
August 24-25, 2010

Walt Polansky



Recovery.gov is the U.S. government's official website that provides easy access to data related to Recovery Act spending and allows for the reporting of potential fraud, waste, and abuse.

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THE RECOVERY ACT

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On Feb. 13, 2009, Congress passed the American Recovery and Reinvestment Act of 2009 at the urging of President Obama, who signed it into law four days later. A direct response to the economic crisis, the Recovery Act has three immediate goals:

- Create new jobs and save existing ones
- Spur economic activity and invest in long-term growth
- Foster unprecedented levels of accountability and transparency in government spending

Project Operating Plans (POP)

Public Benefit & Impact

Cost & Schedule

Milestones (including Quarterly briefs to ASCAC)

Performance Measures

Management (Linkage to DOE Priorities)

All funds must be obligated (out of DOE) by Sept 30, 2010

All funds must be spent by Sept 30, 2015 – unspent funds returned to US Treasury

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Recovery and Reinvestment Act Projects

ASCR's Recovery Act Projects (\$154.9M)

- Advanced Networking Initiative (\$66.8M)
 - Testbed to demonstrate and build tools for 100Gbps optical networking technologies
- Leadership Computing Facility Upgrades (\$19.9M)
 - Six-core upgrade to Oak Ridge LCF machine delivered 2.2 Petaflops
- Advanced Computer Architectures (\$5.2M)
 - Research on next generation technologies
- Magellan (\$33M)
 - Research to demonstrate and build tools to enable scientists to utilize cloud computing resources for mid-range computing needs
- SciDAC-e (\$30M)
 - Supplement and leverage existing SciDAC investments to advance the high performance computational capabilities of the BES - Energy Frontier Research Centers; Extra user support for Energy related projects at the Leadership Computing and NERSC facilities; Applied mathematics research in support of DOE electricity grid efforts.



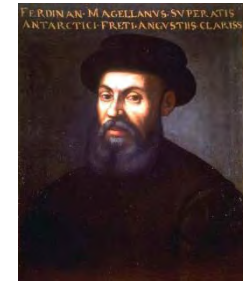
DOE Explores Cloud Computing

- **ASCR Magellan Project Summary**

- \$32M project at NERSC and ALCF
- ~100 TF/s compute cloud testbed (across sites)
- Petabyte-scale storage cloud testbed

- **Project Progress**

- **ANL and LBNL receiving stage II hardware**
 - Flash storage, big memory, GPGPU, 100 Gbps connection to ANI prototype network
- **Completed cross-site demo with single application using both Magellan sites**
- **Regular telecon and on-site meetings to coordinate activities at both sites**
- **Implemented 4 cloud environments**
 - Batch, Virtual Machine, Hadoop, private cluster
- **Science communities actively submitting jobs**
 - 15 M core-hours allocated



- **Cloud questions to explore on Magellan:**

- Can a cloud serve DOE's mid-range computing needs?
 - More efficient than cluster-per-PI model
- What part of the workload can be served on a cloud?
- What features (hardware and software) are needed of a "Science Cloud"? (Eucalyptus at ALCF; Linux at NERSC)
- How does this differ, if at all, from commercial clouds?



ANI: Advanced Network Initiative

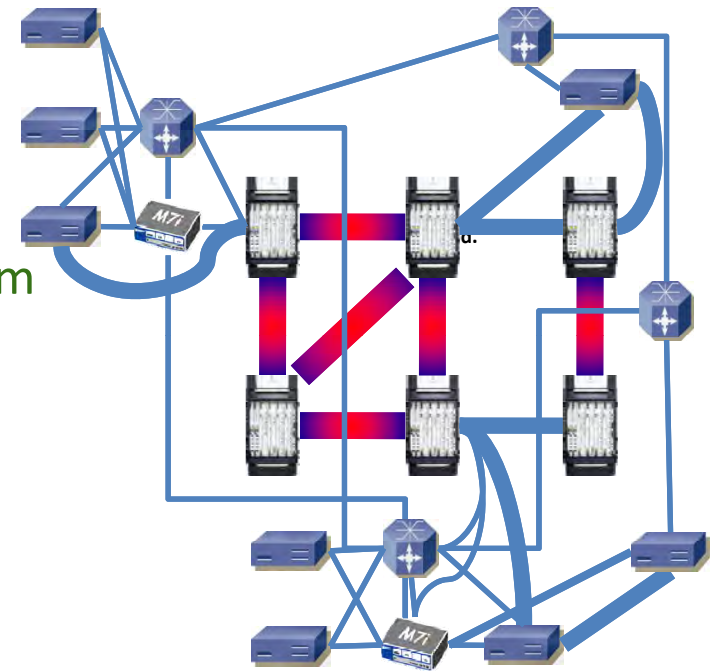
Goals:

- **Accelerate the commercialization of 100 Gigabit per second (Gbps) networking technologies by deploying a national-scale prototype network that will span four distinct geographic regions, connecting the three major ASCR computing facilities and the New York multi-agency peering point providing transatlantic Research and Education (R&E) connectivity at 100 Gbps.**
- **Complement the prototype 100 Gbps network with a testbed providing an experimental network research environment at sufficient scale to usefully test experimental approaches to next generation networks and applications.**



ANI Status

- **Testbed operational as of June 2010**
 - 3 research projects active
 - 3 more waiting for 40 Gbps capability
 - User guide written and basic reservation system in use
- **National 100 Gbps backbone RFP evaluation underway**
 - alpha HW from 3 vendors has been evaluated
- **Process in place to evaluate new research proposals**
 - 1st round due Oct 2010
 - Awards will be made Jan 2011
 - Review committee contains Lab, Academic, Industry, and International members
 - New awards on 6 month time frame



SciDAC-e

- **\$30M ARRA Activity**
- **One time stimulus of applied mathematics & computer science research efforts to establish computational foundation to advance the DOE mission across a wide range, including developing renewable energy sources and developing smart grids.**
- **Implementation Strategy**
 - **Applied mathematics research to enable bigger, better and smarter electricity grids**
 - **Supplemental awards to existing SciDAC efforts to support collaborative research with BES-supported Energy Frontier Research Centers to develop a high-performance computing capability relevant to the goals of the EFRC**
 - **Enhanced user support at NERSC, ALCF & OLCF for SciDAC-e and energy users awarded allocations through ASCR Leadership Computing Challenge allocation process; SciDAC-e summer school for training and experience with Leadership computing resources.**



SciDAC-e: Applied Mathematics

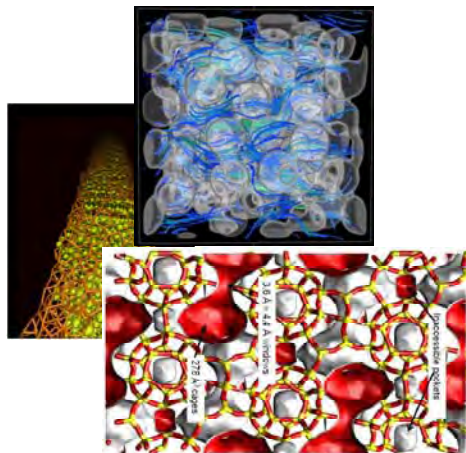
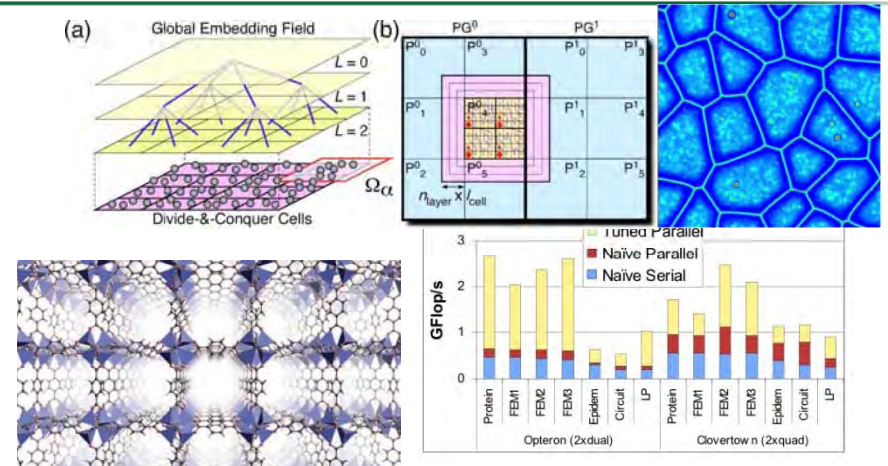
- **Goal: Support of DOE electricity grid efforts.**
 - *Robust Optimization for Connectivity and Flows in Dynamic Complex Networks*, Lead PI: Balasundaram (Oklahoma State)
 - *Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms*, Co-PIs: Bienstock (Columbia), Wright (UW-Madison)
 - *Approaches for Rare-event Simulation and Decision Making*, Lead PI: Shortle (GMU)
 - *Analysis and Reduction of Complex Networks under Uncertainty*, Marzouk (MIT), Knio (JHU), Ghanem (USC), Najm (SNL)
 - *Optimization and Control of the Electric Power Systems*, Co-PIs: Meza (LBNL), Thomas (Cornell), Lesieutre (UW-Madison)
 - *Advanced Kalman Filter for Real-Time Responsiveness in Complex Systems*, Co-PIs: Huang (PNNL), Welch (UNC-Chapel Hill)
 - *Extending the Realm of Optimization for Complex Systems: Uncertainty, Competition and Dynamics*, Lead PI: Shanbhag (UIUC)
- **All awards made; research is underway.**



SciDAC-e: EFRC- SciDAC Collaborations

Supplemental awards to SciDAC Centers and Institutes to enable BES-supported Energy Frontier Research Centers (EFRCs) to develop a high-performance computing capability relevant to the goals of the EFRC

- 14 awards- APDEC, VACET, IUSV, TOPS, ITAPS, PERI, SDM



EFRC Category	# Unique EFRCs	# EFRC Collaborations	Award (\$K)
Materials Under Extreme Conditions	2	3	1,095
Geological Flows & Carbon Storage	3	6	3,931
Solar & Photovoltaics	5	5	3,379
Material Design	1	2	951
Others	4	4	1,540
TOTAL	15	20	10,895



SciDAC-e: Computational Post-Docs

- Enhance user support, via two-years of funding (\$10M total funding) for approximately 30 new Postdoctoral Appointments at ASCR facilities.
- Provide expert assistance to SciDAC-e projects and other energy users awarded allocations through the ASCR Leadership Computing Challenge (ALCC) allocation process.
- Through a SciDAC-e summer school, provide projects with training and hands on experience with Leadership computing resources.
- NERSC (\$3.125M); ALCF (\$3.125M); OLCF (\$3.75M)



SciDAC-e: ALCF Postdoc Summary

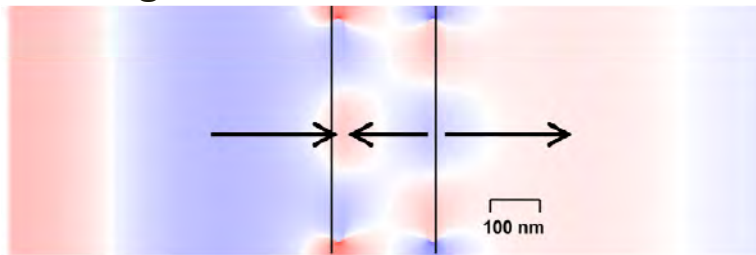
- **Staffing**
 - Hired 11
 - 6 on-board; 5 starting in next 6 months (3 MCS, NE, MSD)
- **Science Insight**
 - Negative Index Materials (NIM) calculations scaling to as many as 32 racks of the Blue Gene/P system have resulted in metamaterial structures which we predict to have figures of merit (a measure of the quality of the NIM) that are nearly double the values of related structures reported in literature.
 - Extended Hamiltonian replica-exchange MD (H-REMD) simulation method with an accelerated MD method to overcome problems arising from the existence of kinetically trapped conformations within the protein receptor.



SciDAC-e: ALCF Posdoc Highlights

E. DePrince – Metamaterials (Computational Materials Science)

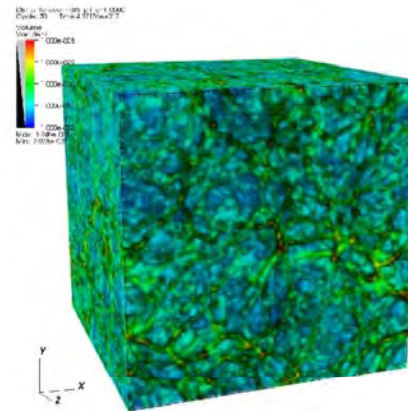
- Computational studies of materials that can exhibit a range of unique electromagnetic properties such as having negative-index of refraction
- Potential applications including imaging beyond the diffraction limit and optical cloaking



Finite-difference time-domain (FDTD) simulation showing the electric field patterns for a two-dimensional negative index material (NIM) consisting of two gold rods separated by SiO₂. The arrows show the direction that the light "appears" to be propagating inside and outside of the NIM

J. Bernstein – Dark Energy (Computational Hydrodynamics & Cosmology)

- Radiative transfer calculations for thermonuclear supernova (SN Ia) simulations
- N-body + hydrodynamic (computational cosmology) simulations of the large scale structure of the Universe



Rendered results of a dark energy simulation run on an ALCF resource. The density variable is represented for the large-scale structure simulation with 512³ dark matter particles and hydrodynamics enabled.



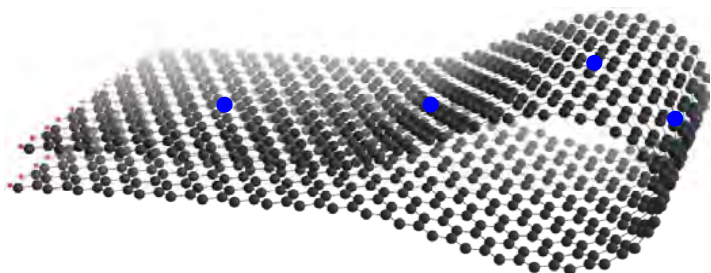
SciDAC-e OLCF Postdoc Summary

- **Staffing**
 - 6 postdocs working; 2 postdocs starting this year
 - 1 offer in progress
 - 1 position vacant due to resignation (Hampton)
- **Science insights**
 - Preliminary results pointing to new chemical method for tailoring the band gap of semiconducting graphene nanoribbons (GNR) (Lopez-Bezanilla)
- **Papers**
 - Paper co-authored by S. Hampton won best paper award at HPCS conference
 - Another paper co-authored by S. Hampton accepted to SC10
- **Code development**
 - LAMMPS kernels identified and ported to GPU (Hampton)
 - Development of LMP2 chemistry code to use MADNESS runtime environment (Mintz)
- **Conferences**
 - HPCS: International Conference on High Performance Computing & Simulation, June 5 – 9, 2010 (Hampton)
 - NT2010: 11th International Conference on the Science and Application of Nanotubes, June 27 – July 2, 2010 (Lopez-Bezanilla)
 - SciApps10 at ORNL, August 3 – 6, 2010 (all postdocs)



SciDAC-e: OLCF Postdoc Highlights

A. Lopez-Bezanilla -- quantum transport in folded graphene nanoribbon (GNR) (Computational Materials Science)



- A linearly-scaling DFT code (SIESTA) is used to perform systematic studies of stable configurations of an N-doped (blue) folded GNR
- These studies will allow one to quantify the conductivity process in chemically modified carbon-based materials, such as new types of electrodes for compact batteries and supercapacitor systems

J. Hursey -- Scalable, Resilient HPC Application & MPI Co-development (Computer Science)

- **Co-development of scalable, resilient HPC applications and MPI fault tolerance extensions allows for:**
 - Development of fault tolerance programming paradigms tailored to application designs, and
 - Quick prototyping and deployment of new MPI semantics influencing the ongoing MPI Forum standardization efforts.
- **Initial work with MADNESS and Open MPI to focus on run-through stabilization, then process recovery**



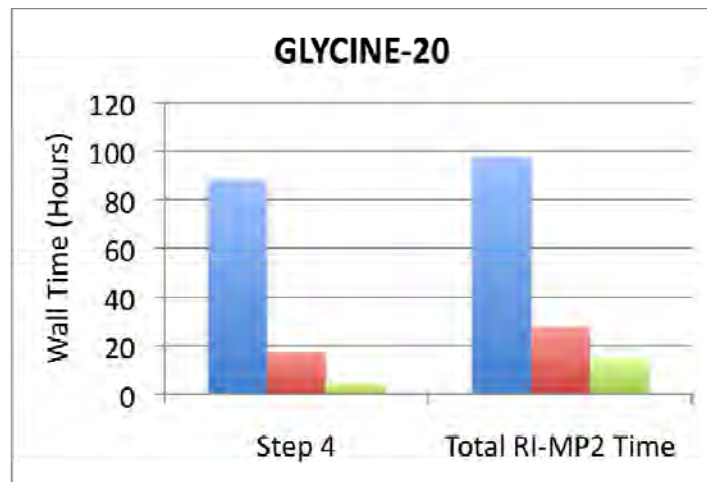
SciDAC-e: NERSC Postdoc Summary

- **Staffing**
 - 8 positions filled with post-docs starting after completing their PhD thesis
 - 5 have started working at NERSC
 - 3 due to start in ~Oct – Nov 2010
 - Another offer has been extended
- **Two post-docs (Kim and Preissl) were co-authors and significant contributors to the paper “Application Acceleration on Current and Future Cray Platforms,” winner BEST PAPER, CUG 2010, Edinburgh, Scotland, May 2010**
- **First Author Conference Poster Presentations were given:**
 - J. Kim, et al. “Calculation of RI-MP2 Gradient using Fermi GPUs”, MQM 2010 (Molecular Quantum Mechanics), Berkeley, CA, May 24 – 29, 2010.
 - R. Preissl, et al., “What’s Ahead for Fusion Computing?,” International Sherwood Fusion Theory Conference, Seattle, WA, April 19 – 21, 2010.
- **Two post-docs (Kim and Maia) served as teaching assistants for the NERSC-sponsored user course on GPUs**
 - Computational Science Summer School, August 2-6, 2010
- **An oral presentation was given by Jihan Kim on July 27, 2010 to the Cray Management team on GPU computing**



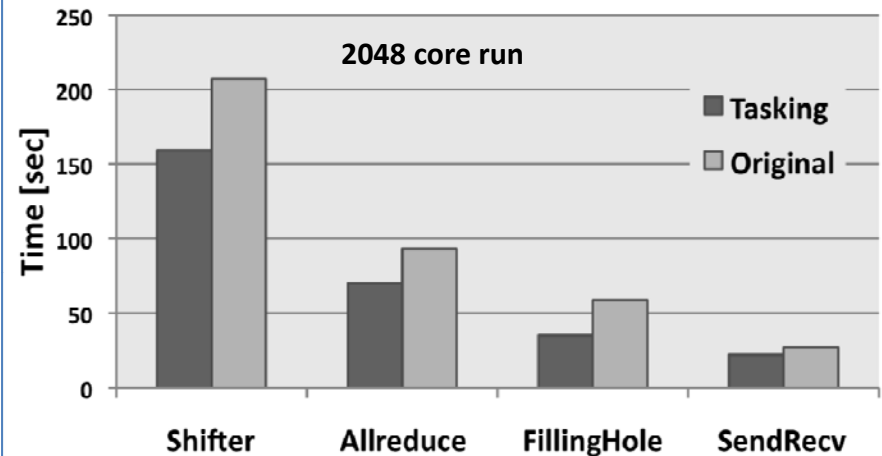
SciDAC-e: NERSC Postdoc Highlights

J. Kim – quantum chemistry code (Q-chem) on GPUs



- Blue: CPU single thread, Red: CPU 2 quad-cores (8 threads), Green: GPU
- CPU: quad-core Intel Nehalem 2.67 GHz, Intel MKL 10.2; GPU: Dirac NERSC cluster (44 Fermi Tesla C2050 GPU cards)
- Glycine-20 Step 4: GPU 18.8x faster than CPU single thread wall time

R. Preissl -- New hybrid tasking model to speed up the GTS code



- New MPI + OpenMP Tasking Model enables us to overlap MPI communication with independent computation and reduce overall runtime by reducing costs of MPI communication.
- Results from NERSC Franklin show performance improvement even on only 4 cores

